

FIG. 1(a)

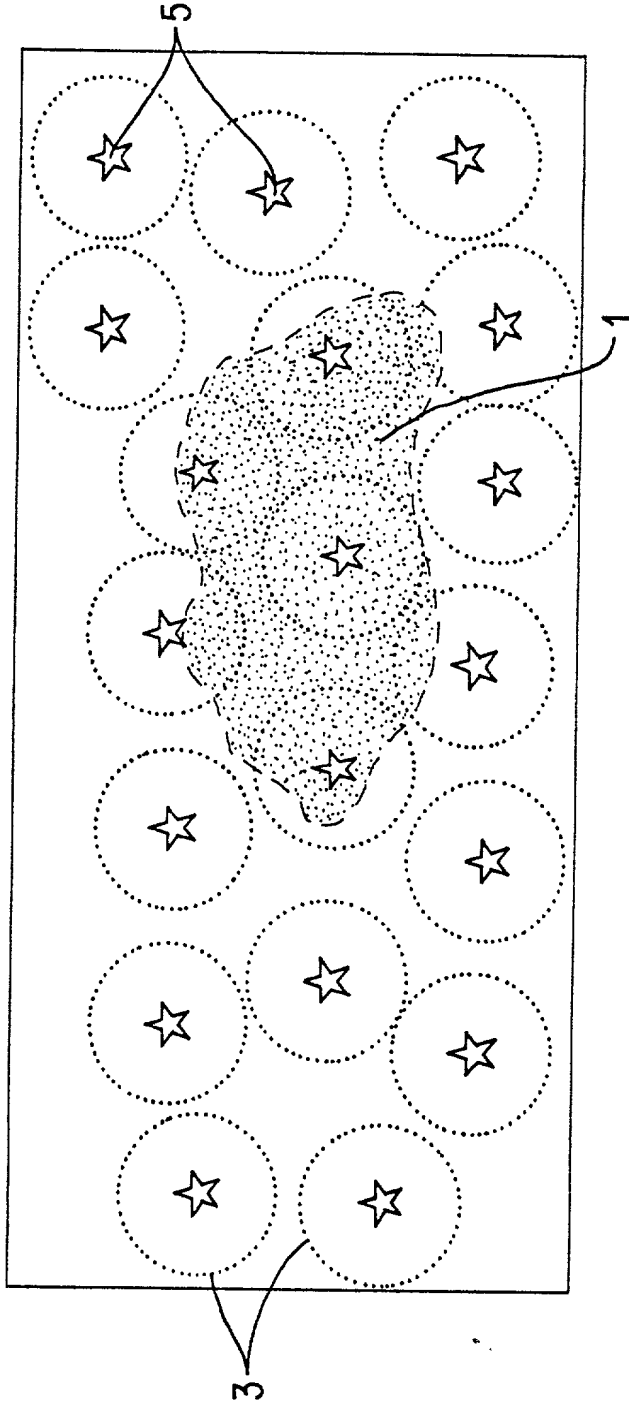


FIG. 1(b)

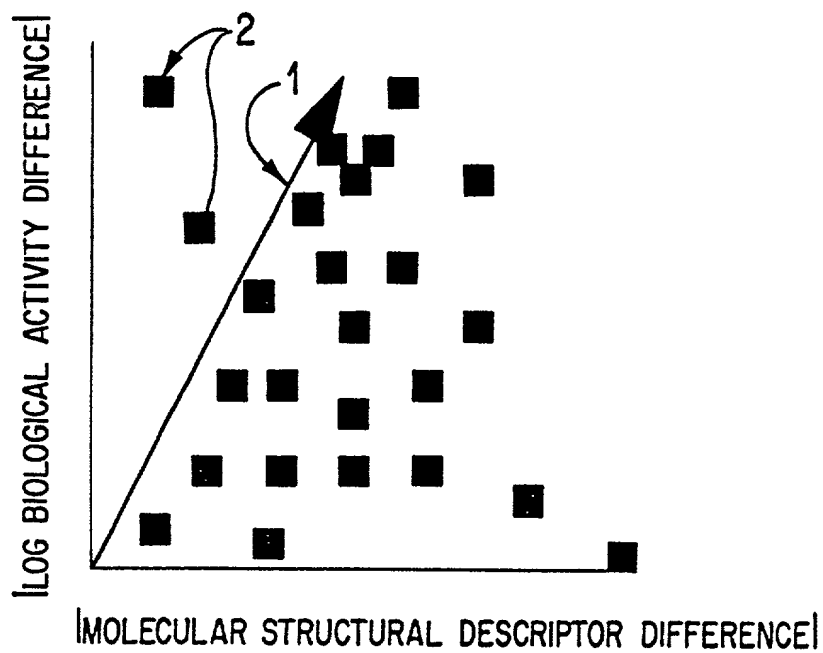


FIG. 2

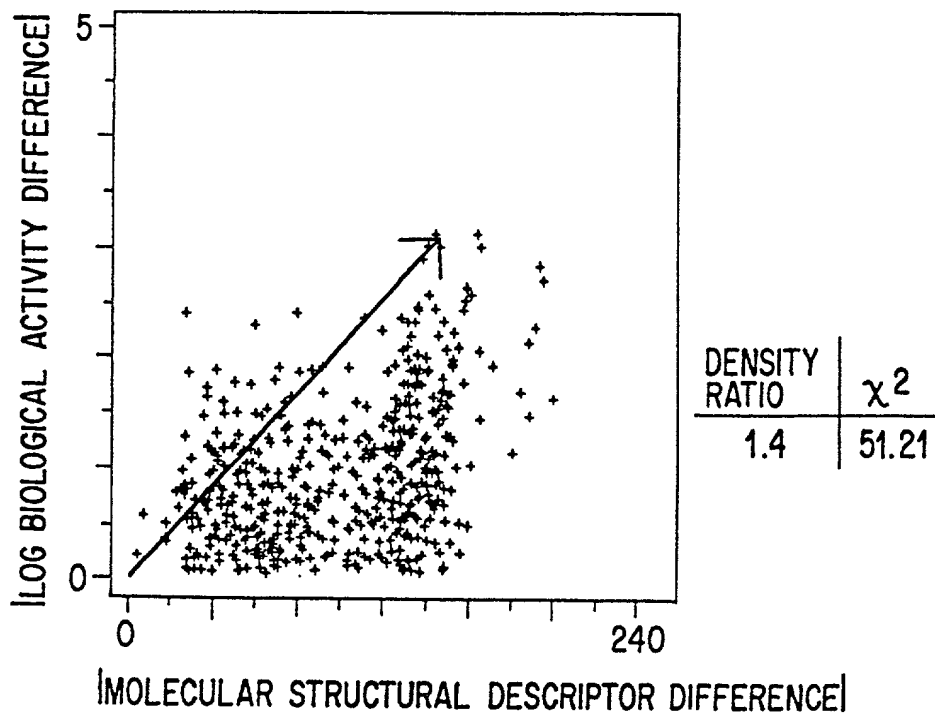


FIG. 3

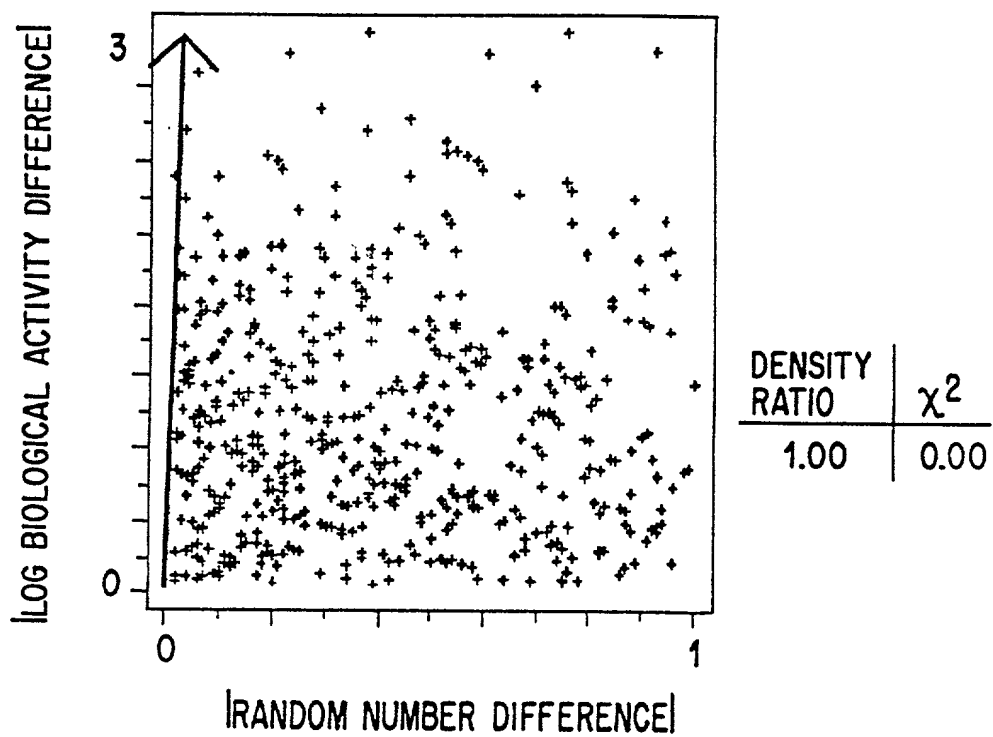


FIG. 4

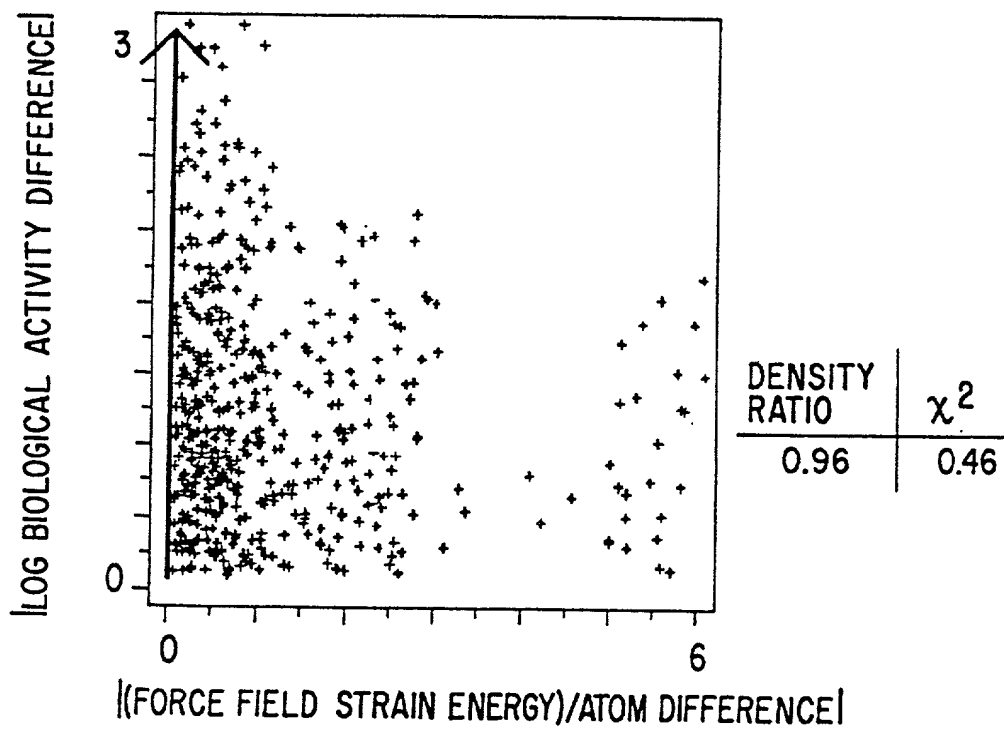
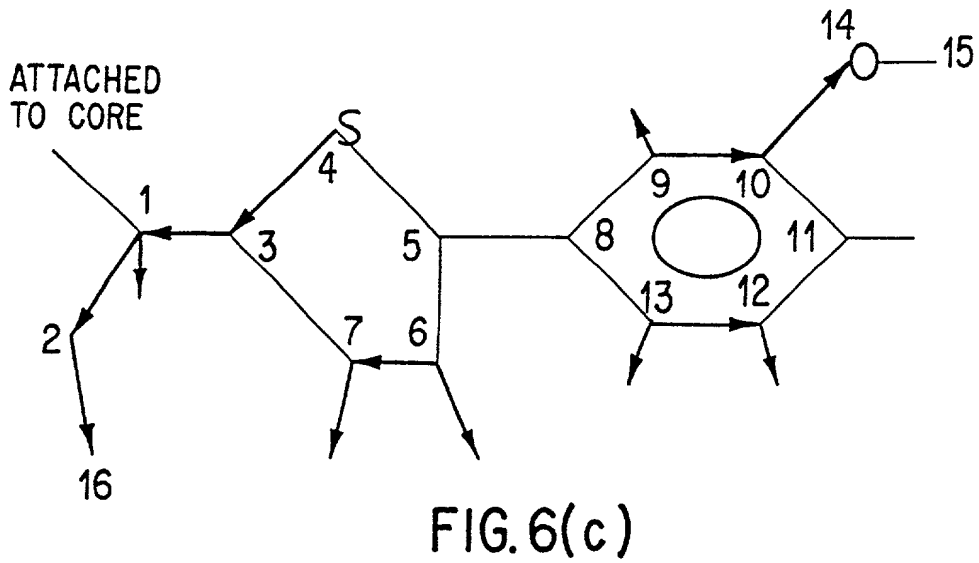
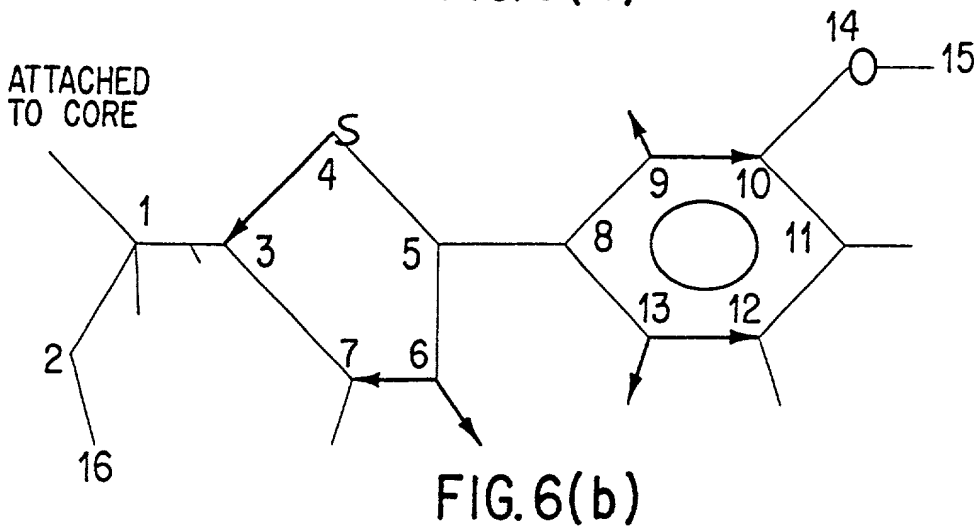
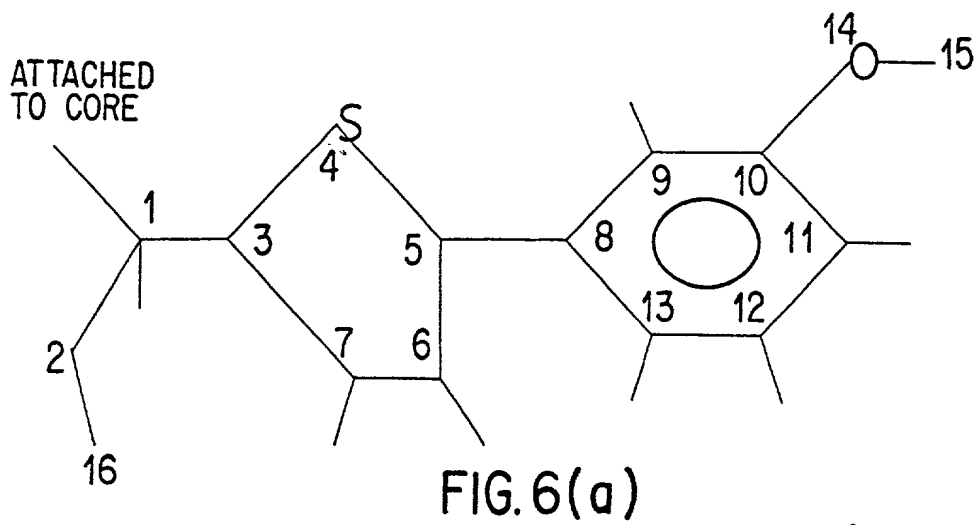


FIG. 5



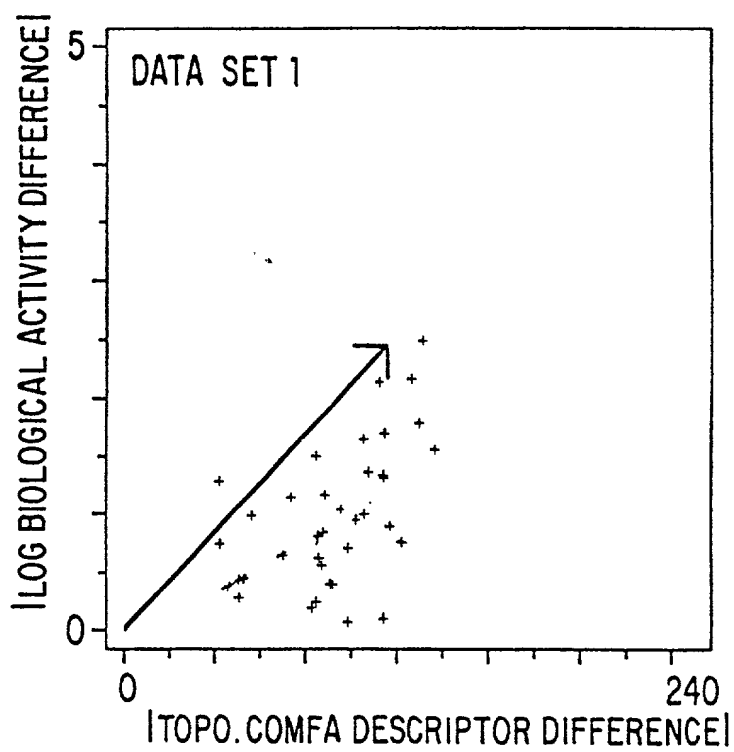


FIG.7(a)

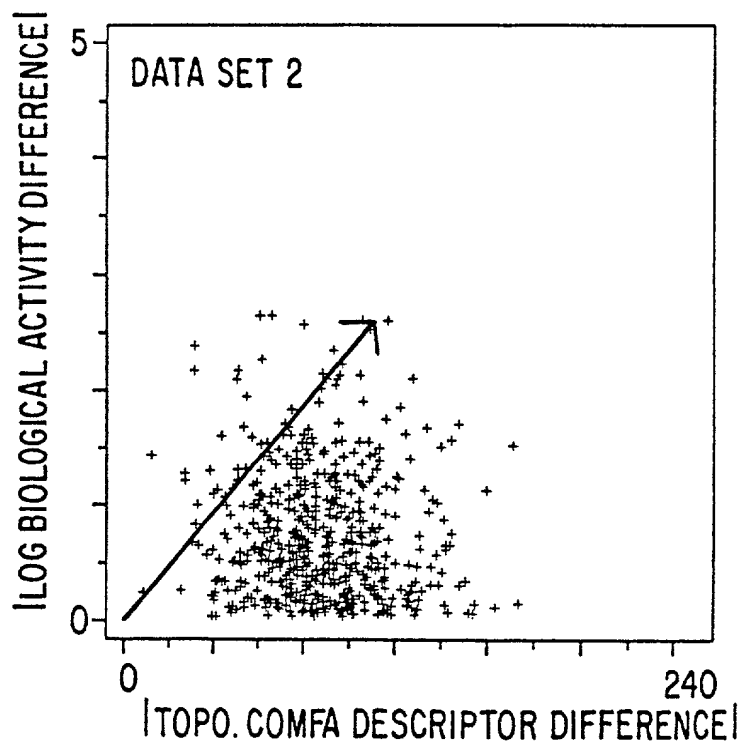


FIG.7(b)

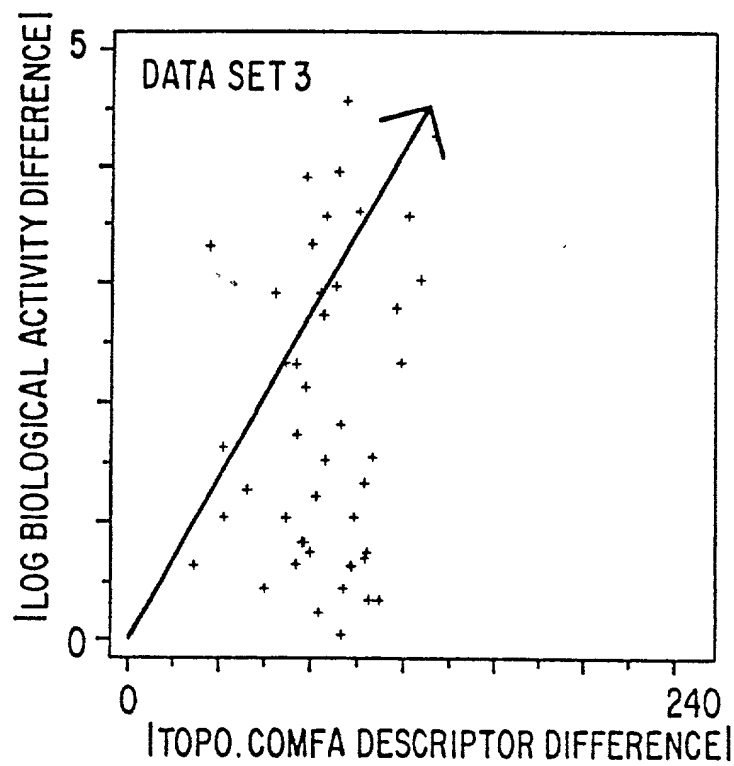


FIG. 7(c)

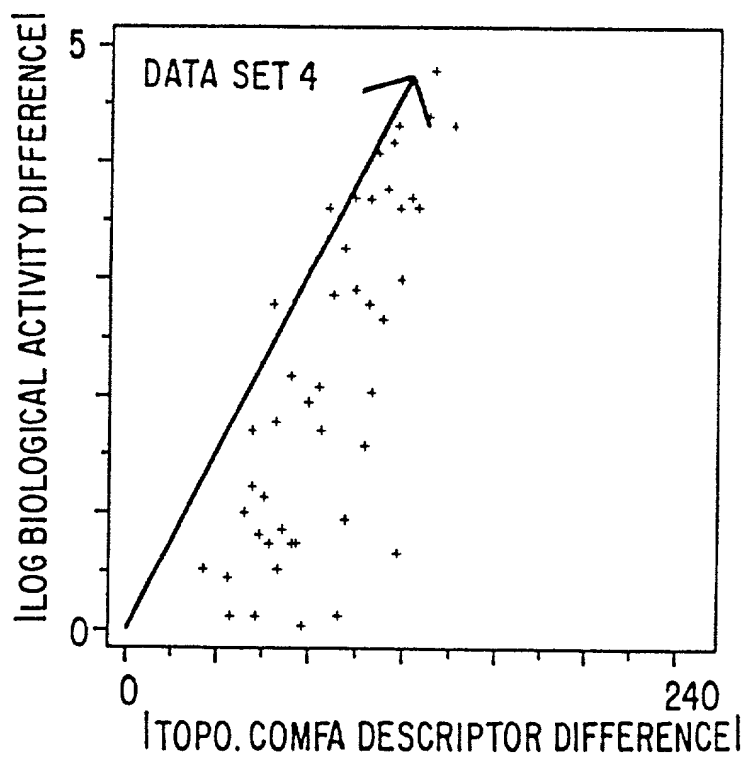


FIG. 7(d)

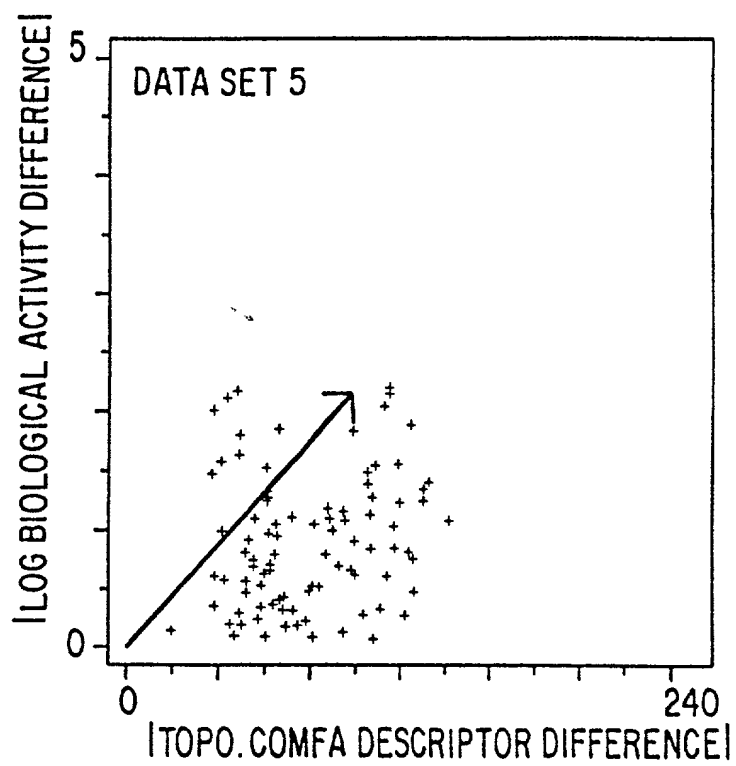


FIG.7(e)

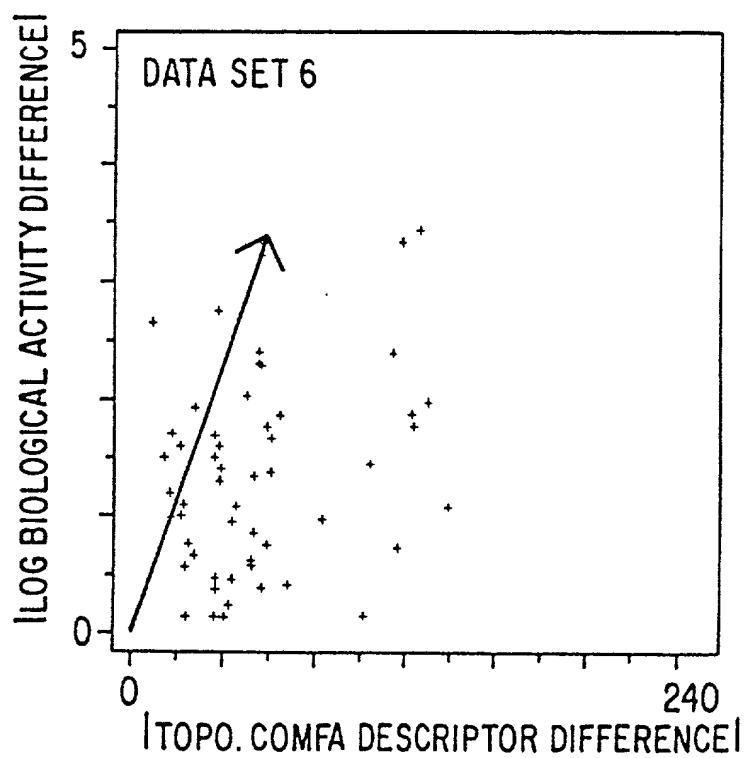


FIG.7(f)



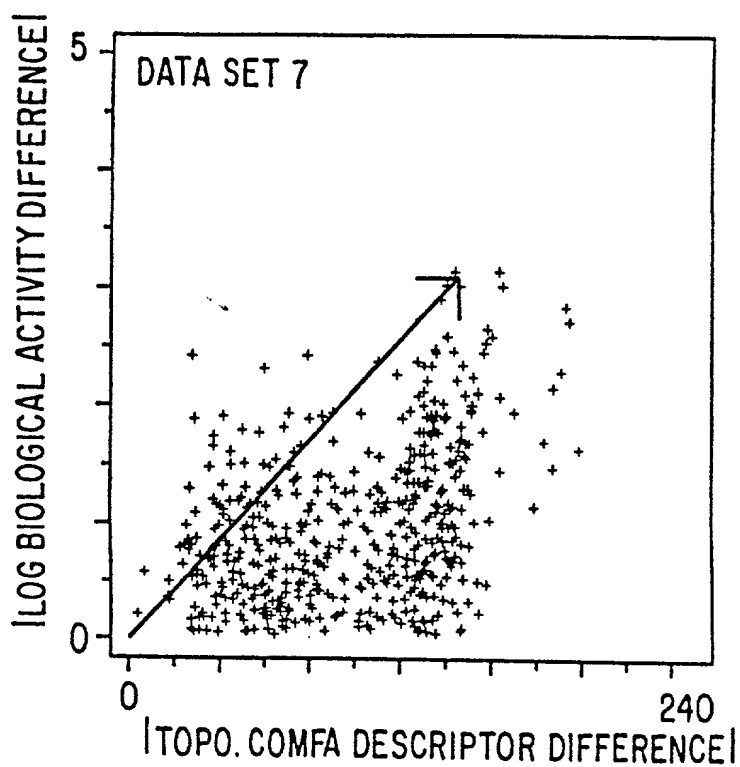


FIG.7(g)

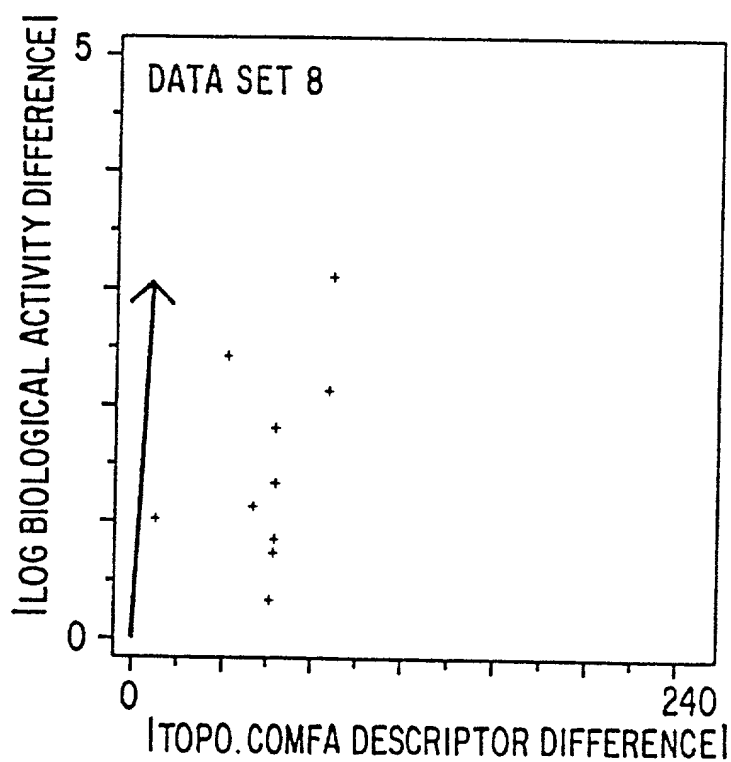


FIG.7(h)

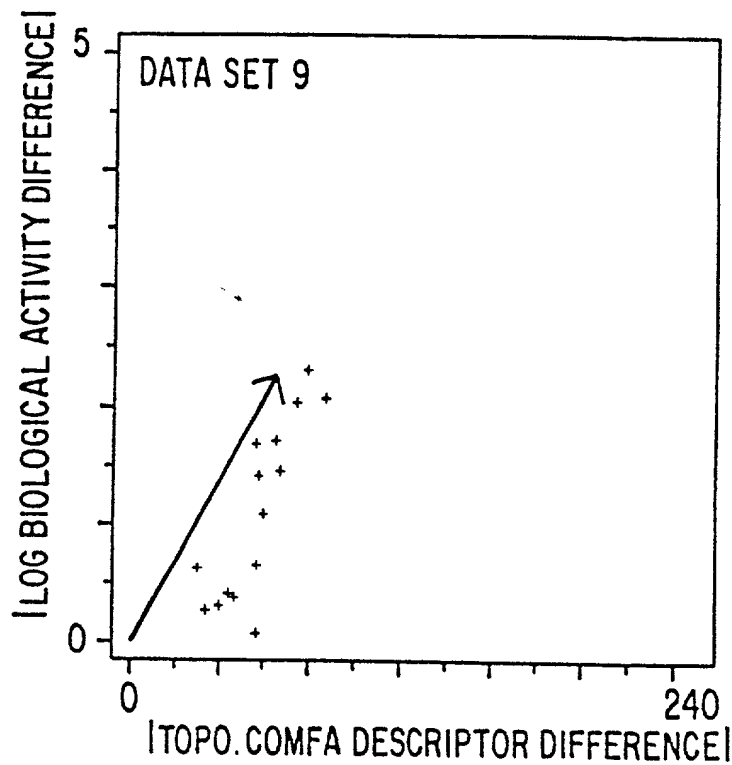


FIG.7(i)

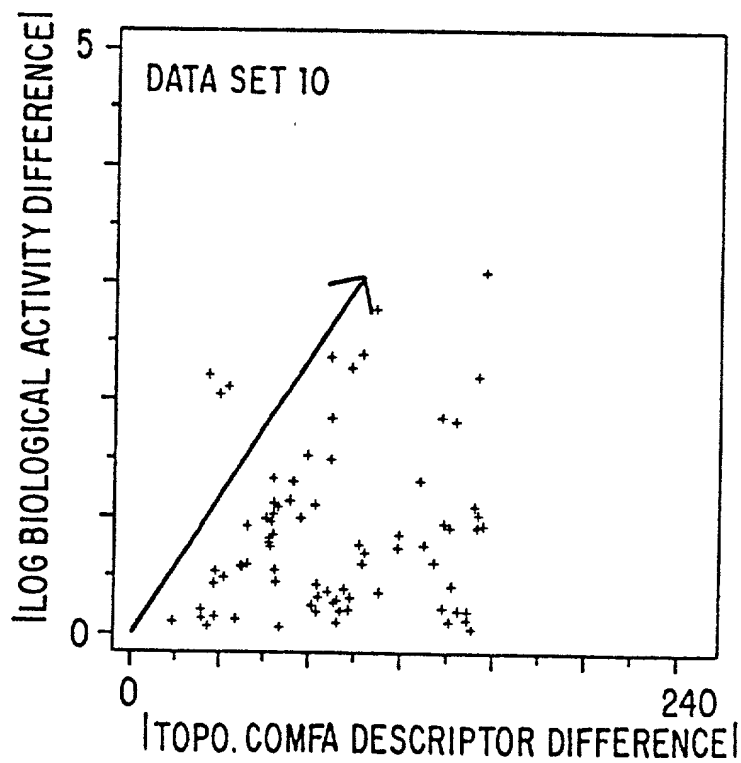


FIG.7(j)

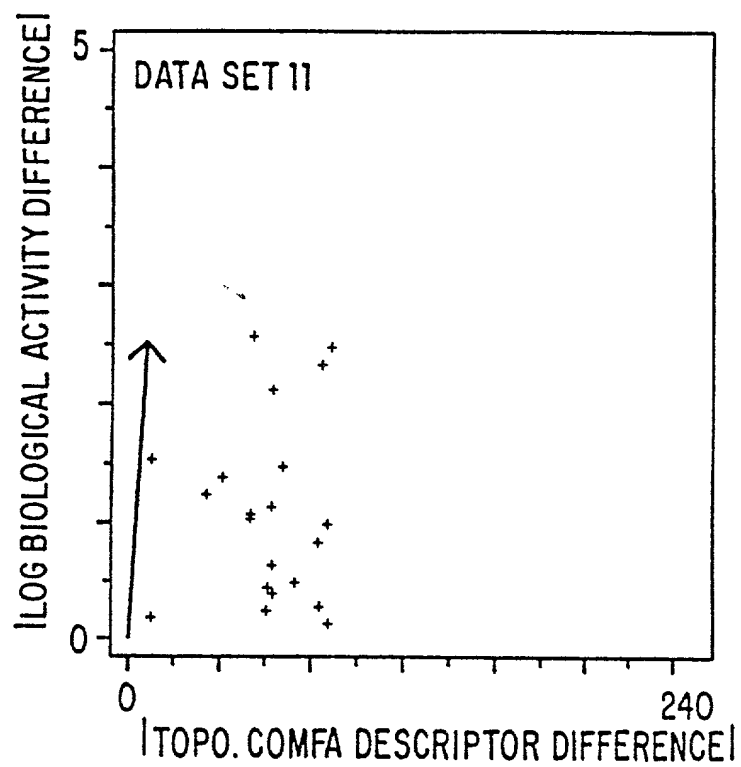


FIG.7(k)

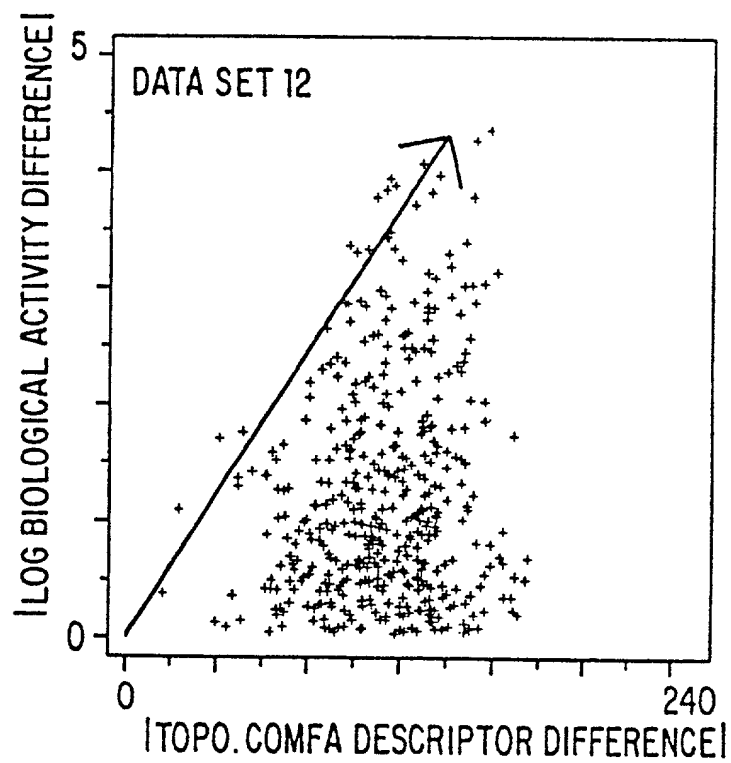


FIG.7(l)

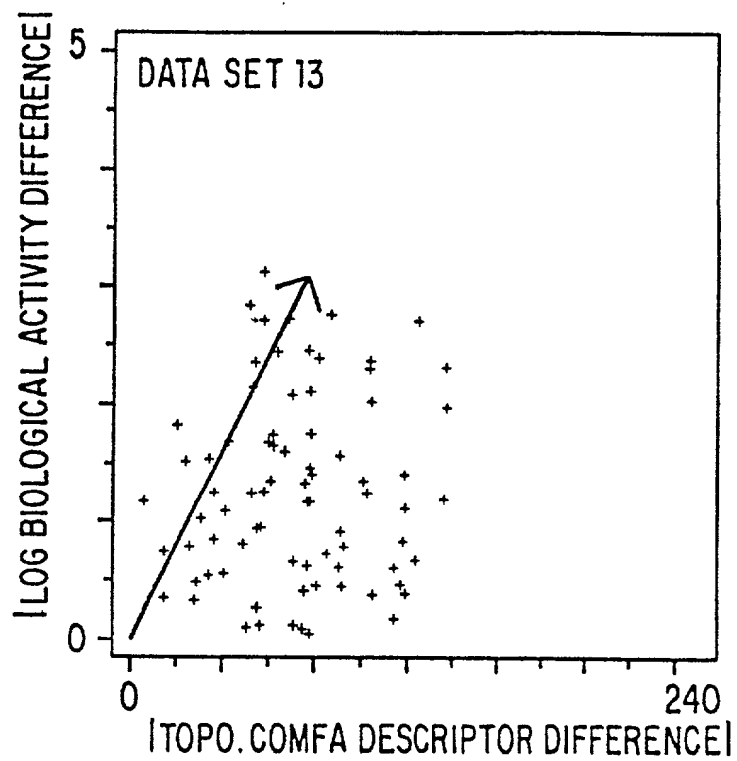


FIG.7(m)

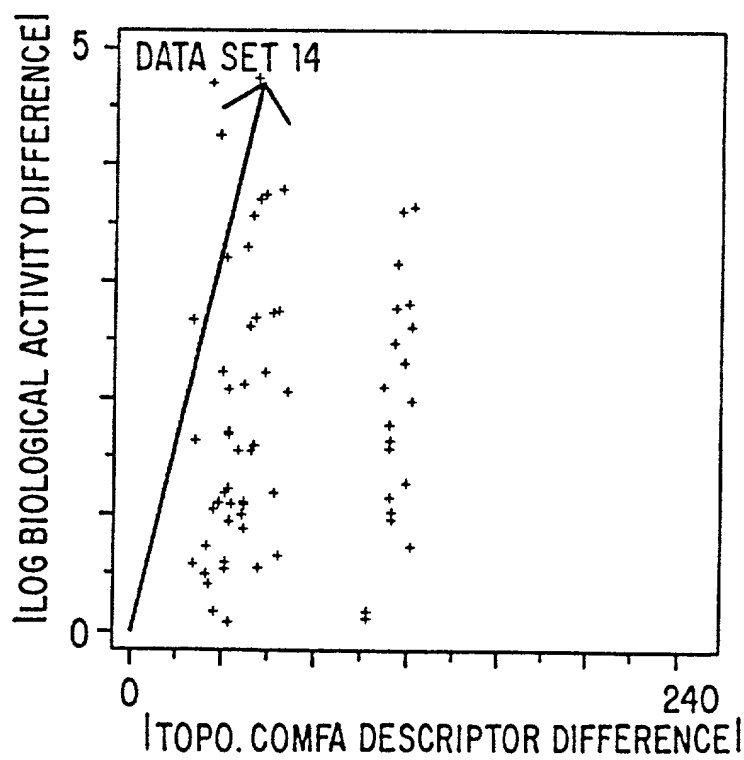


FIG.7(n)

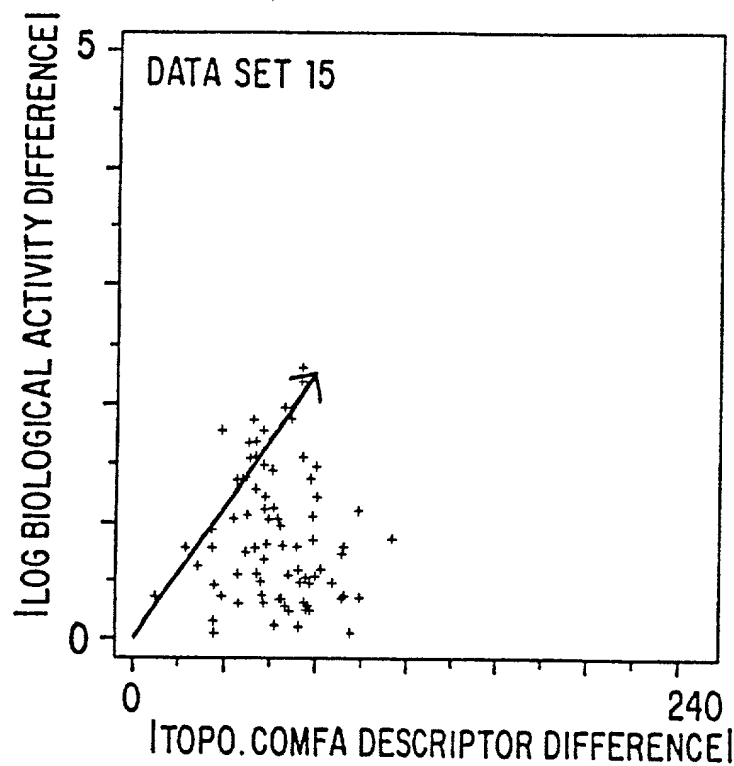


FIG.7(o)

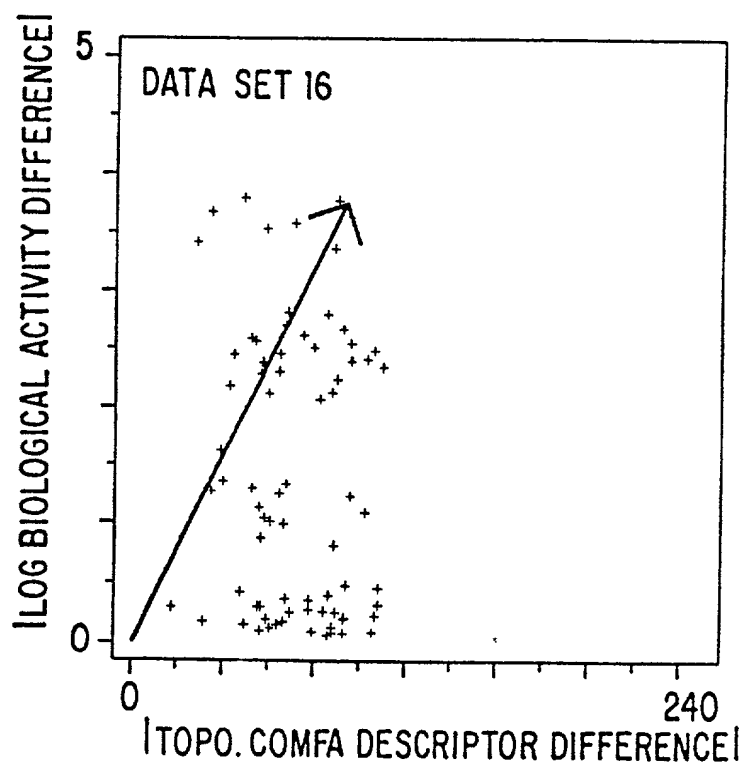


FIG.7(p)

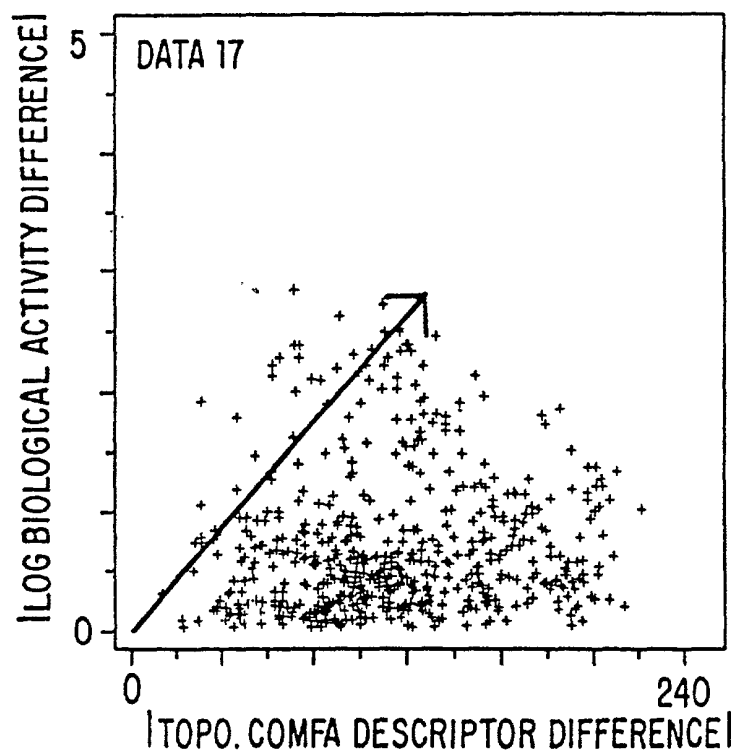


FIG.7(q)

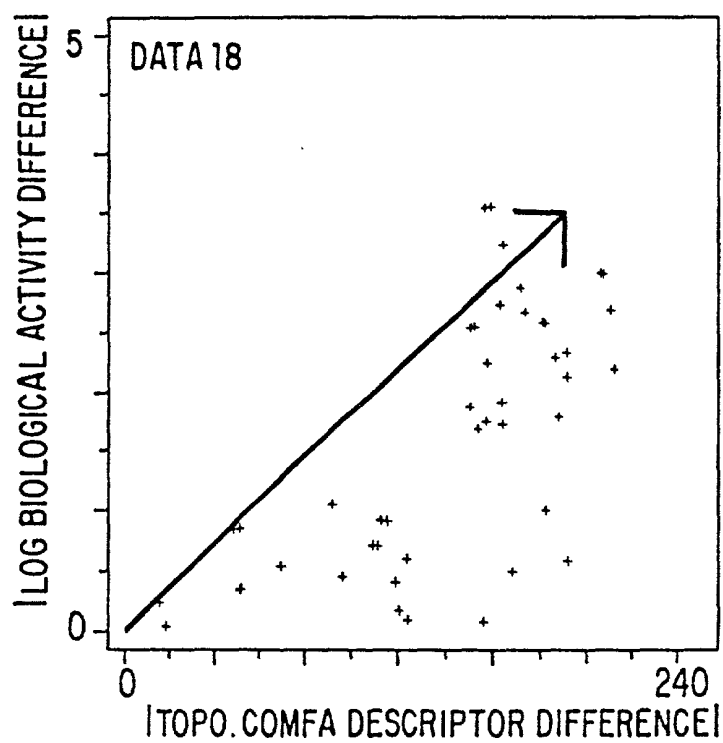


FIG.7(r)

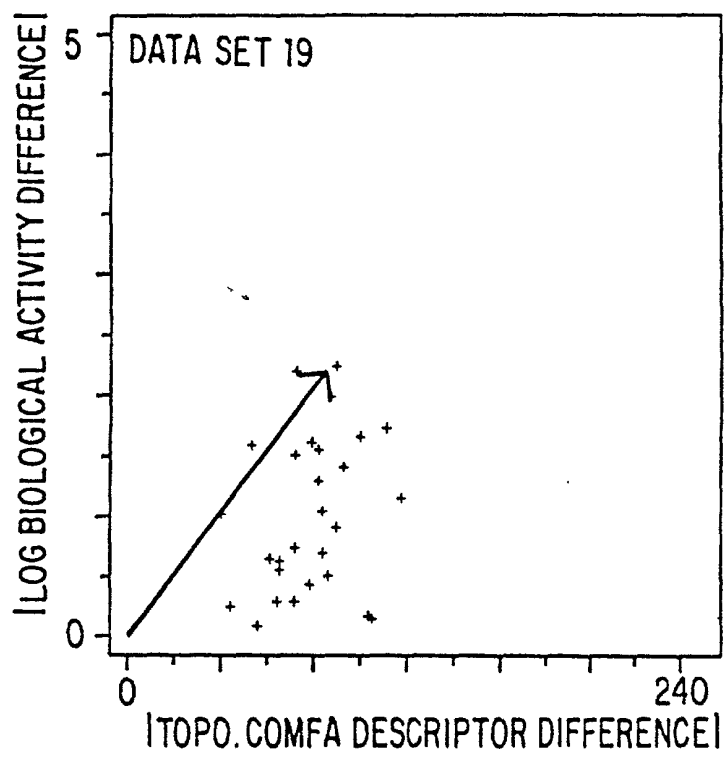


FIG. 7(s)

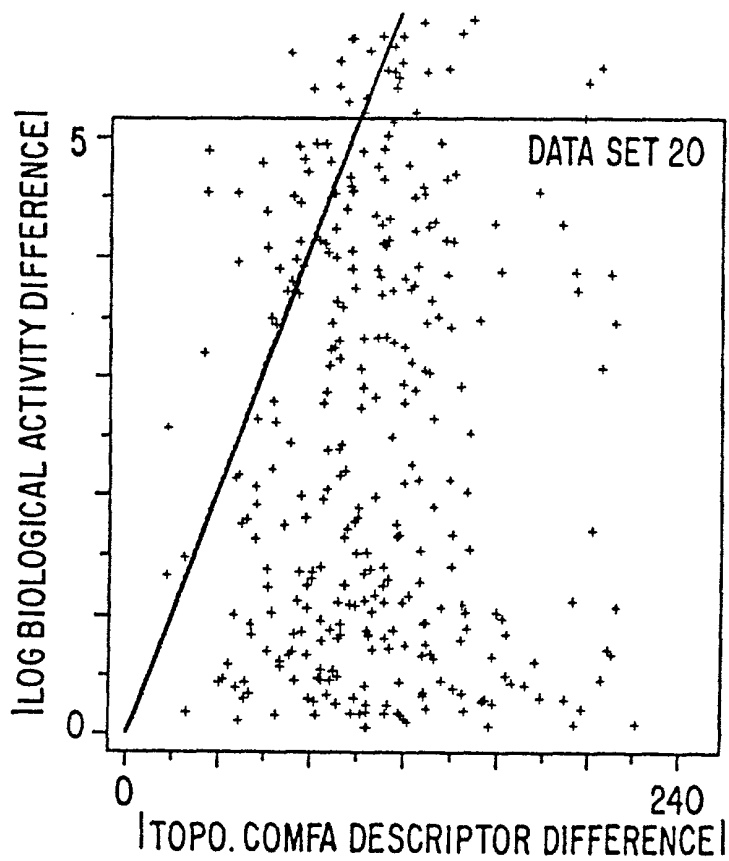


FIG. 7(t)

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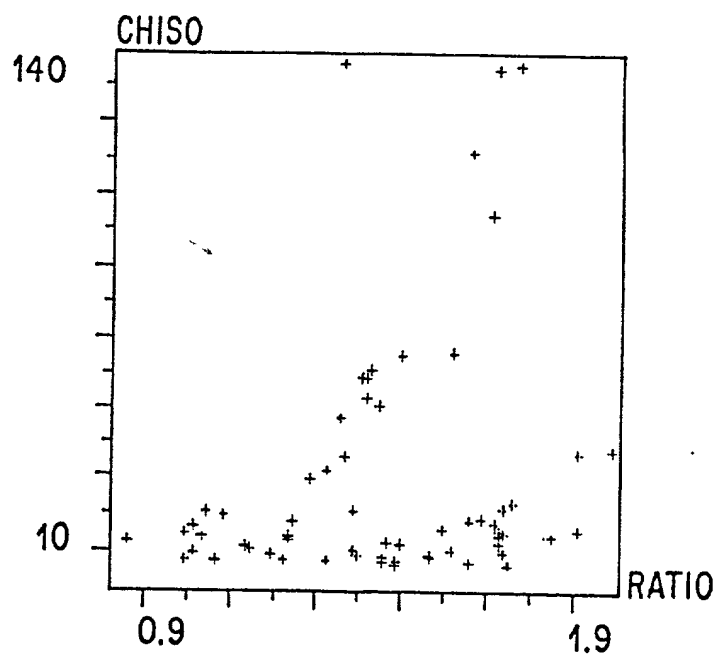


FIG. 8(a)

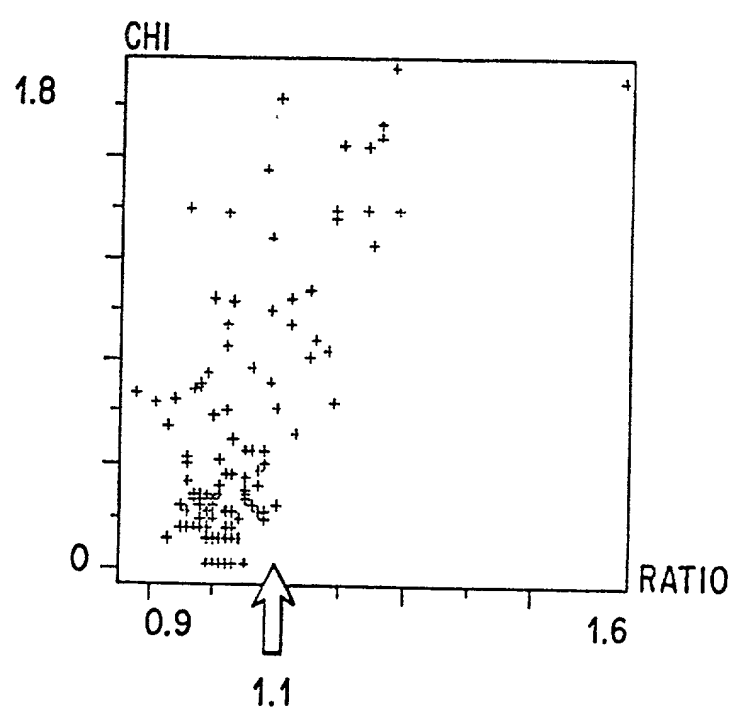


FIG. 8(b)



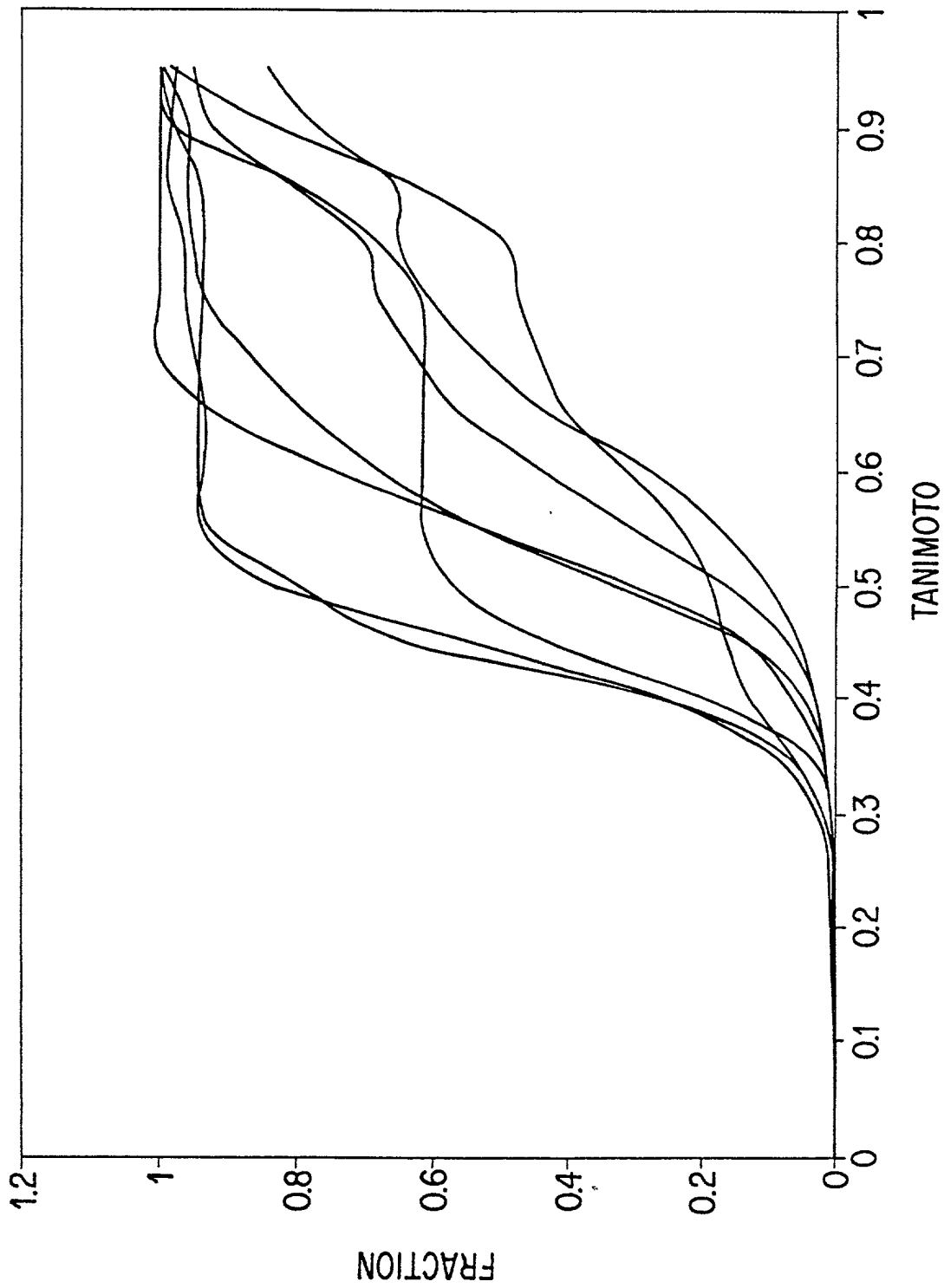


FIG. 9(a)

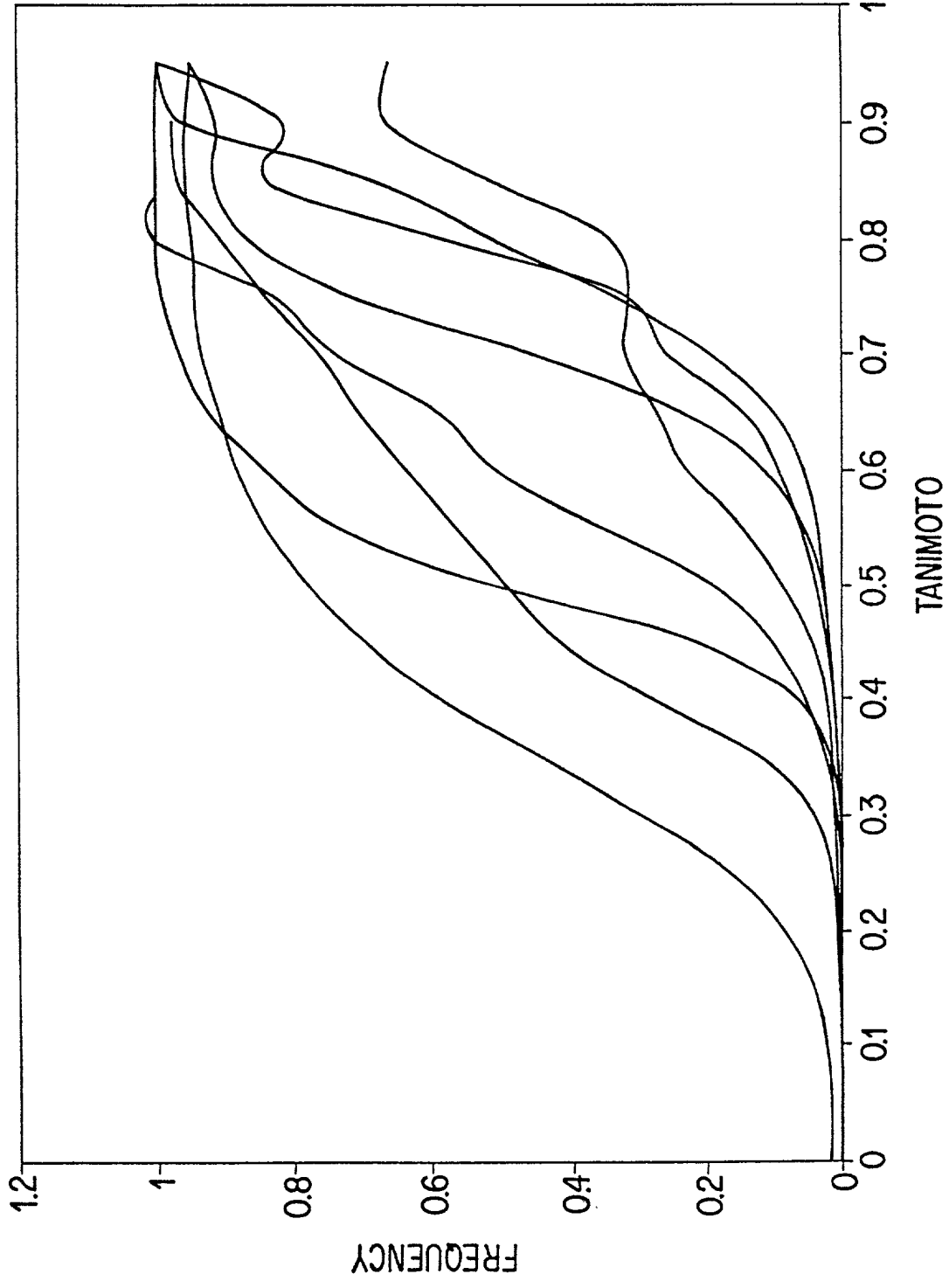


FIG. 9(b)

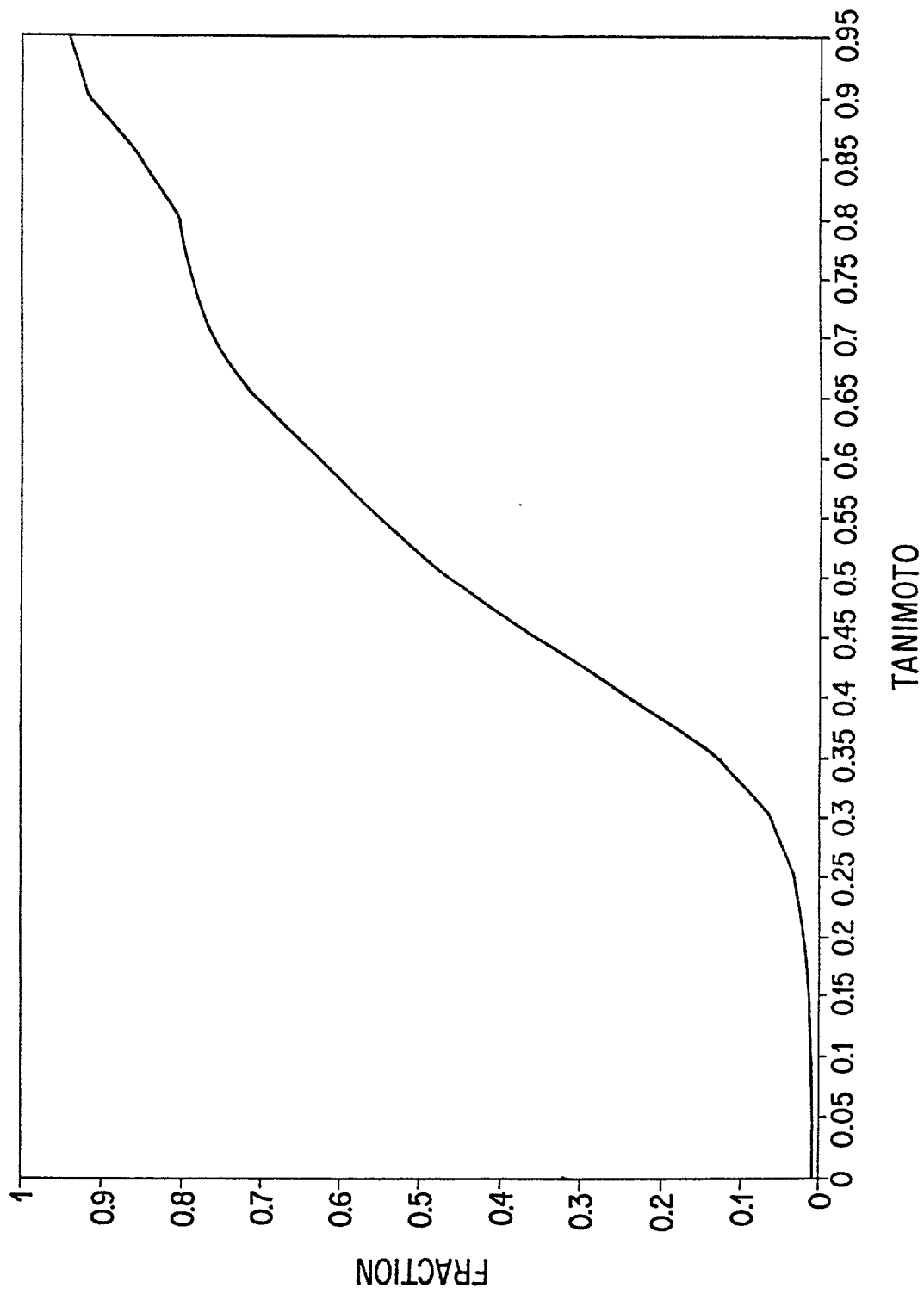


FIG. 9(c)

TOP500-2025-06

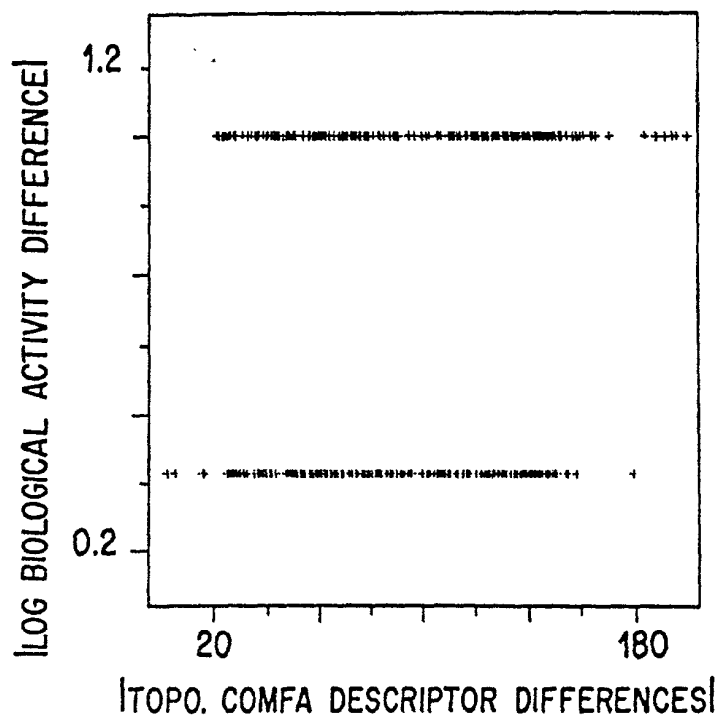


FIG.10(a)

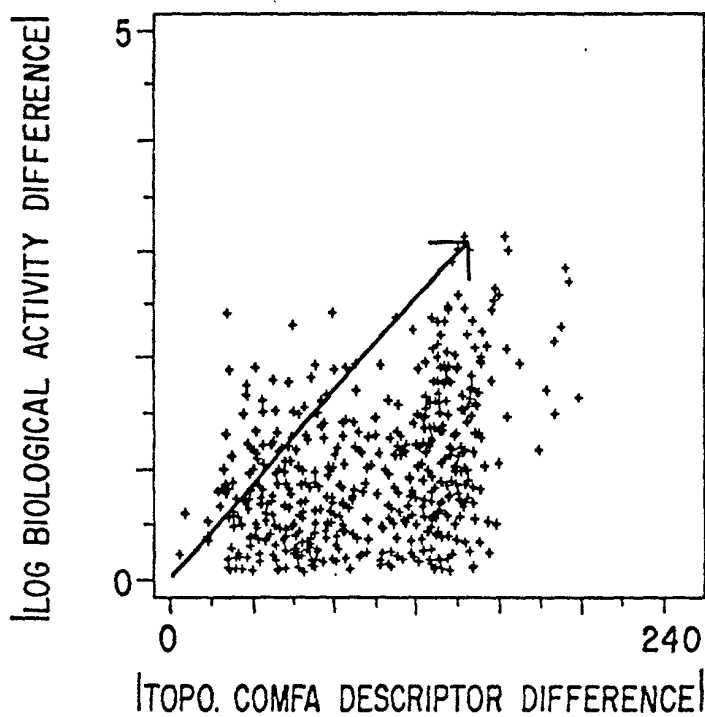


FIG.10(b)

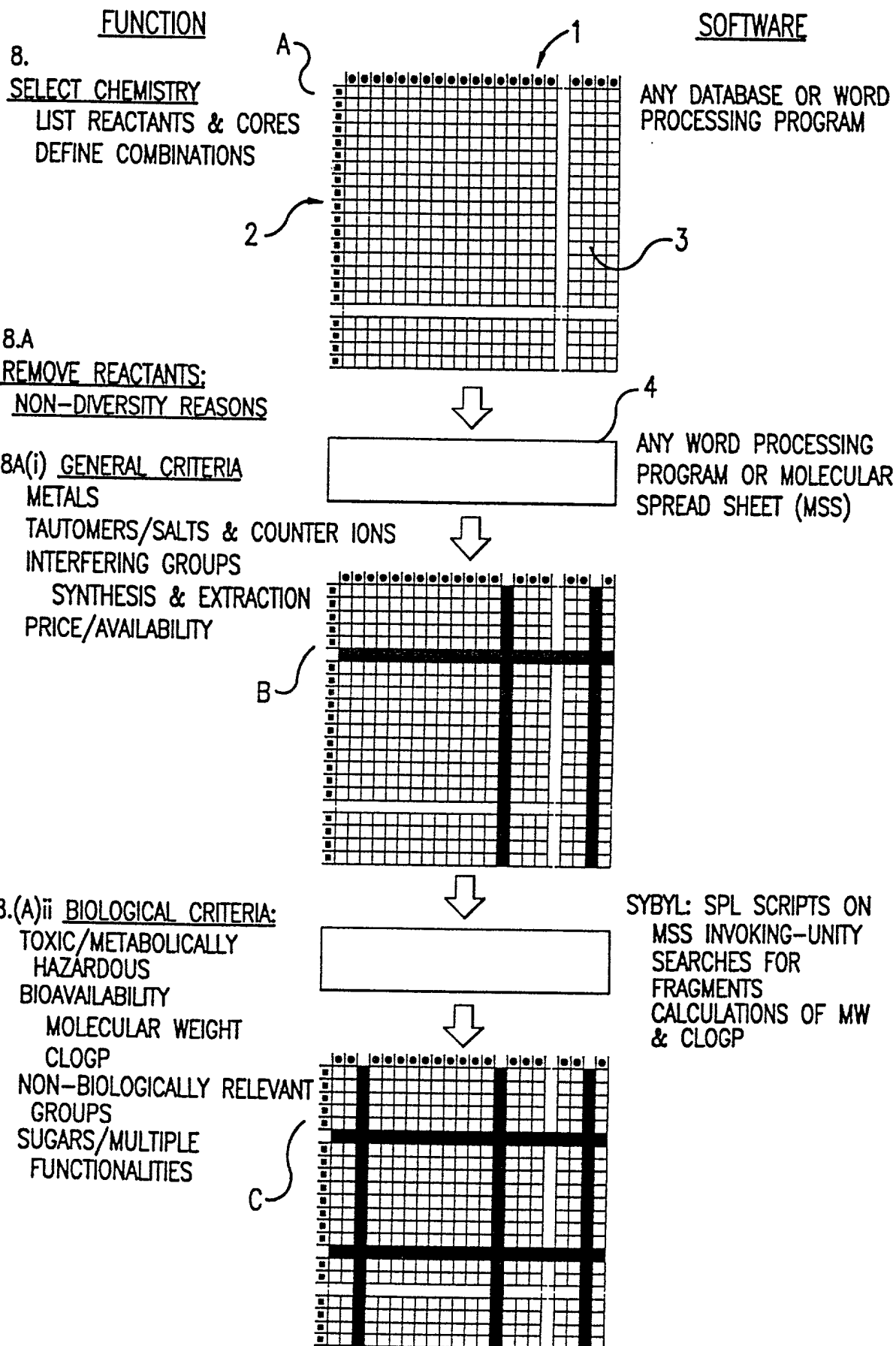
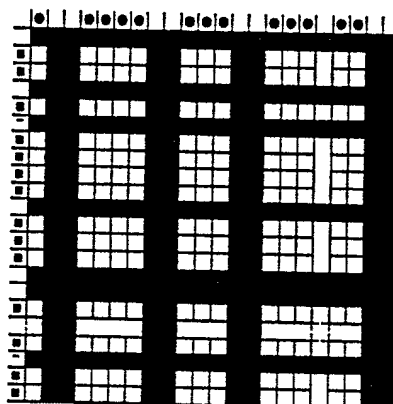


FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION  
 TOPOMERIC CONFORMER  
 ALIGNMENT  
 CoMFA FIELD GENERATION:  
 HYDROGEN BOND FIELD  
 GENERATION  
 ROTATABLE BOND FIELD  
 ATTENUATION  
 CALCULATE FIELD  
 DIFFERENCES  
 CLUSTER  
 REACTANT SELECTION FROM  
 EACH CLUSTER



SYBYL: SELECTOR &  
 CONCORD 3.2.1  
 SPECIALIZED SOFTWARE:  
 APPENDIX "A"  
 (SYBYL: CoMFA  
 STERIC & MSS)

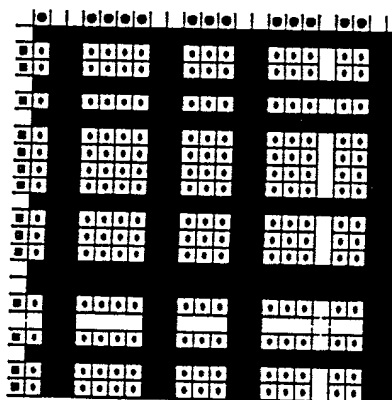
SYBYL: HIERCHICAL  
 CLUSTER - MSS  
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS



E



SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:

NON-DIVERSITY REASONS

GENERAL CRITERIA:



SYBYL: SPL SCRIPTS  
 ON MSS

F

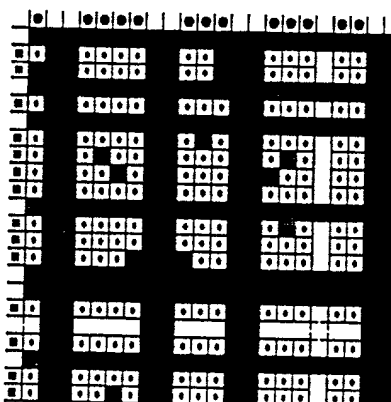


FIG.11(b)

403029-8029260

8D

BIOLOGICAL CRITERIA:

METABOLICALLY HAZARDOUS

BIOAVAILABILITY

MOLECULAR WEIGHT

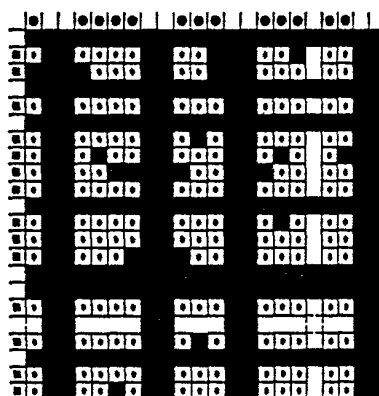
CLOGP

SYBYL: SPL SCRIPTS ON  
MSS INVOKING -

UNITY SEARCHES FOR  
FRAGMENTS

CALCULATIONS OF MW  
& CLOGP

G



8E

REMOVE NON-DIVERSE  
PRODUCTS:

GENERATE TANIMOTO  
2D FINGERPRINTS

SAMPLE PRODUCTS:

EXCLUDE TAN  $\geq 0.85$

UNITY

H

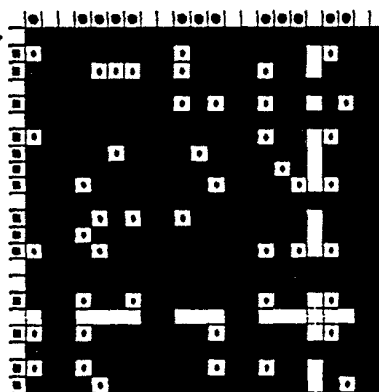


FIG.11(c)

FIG. 12



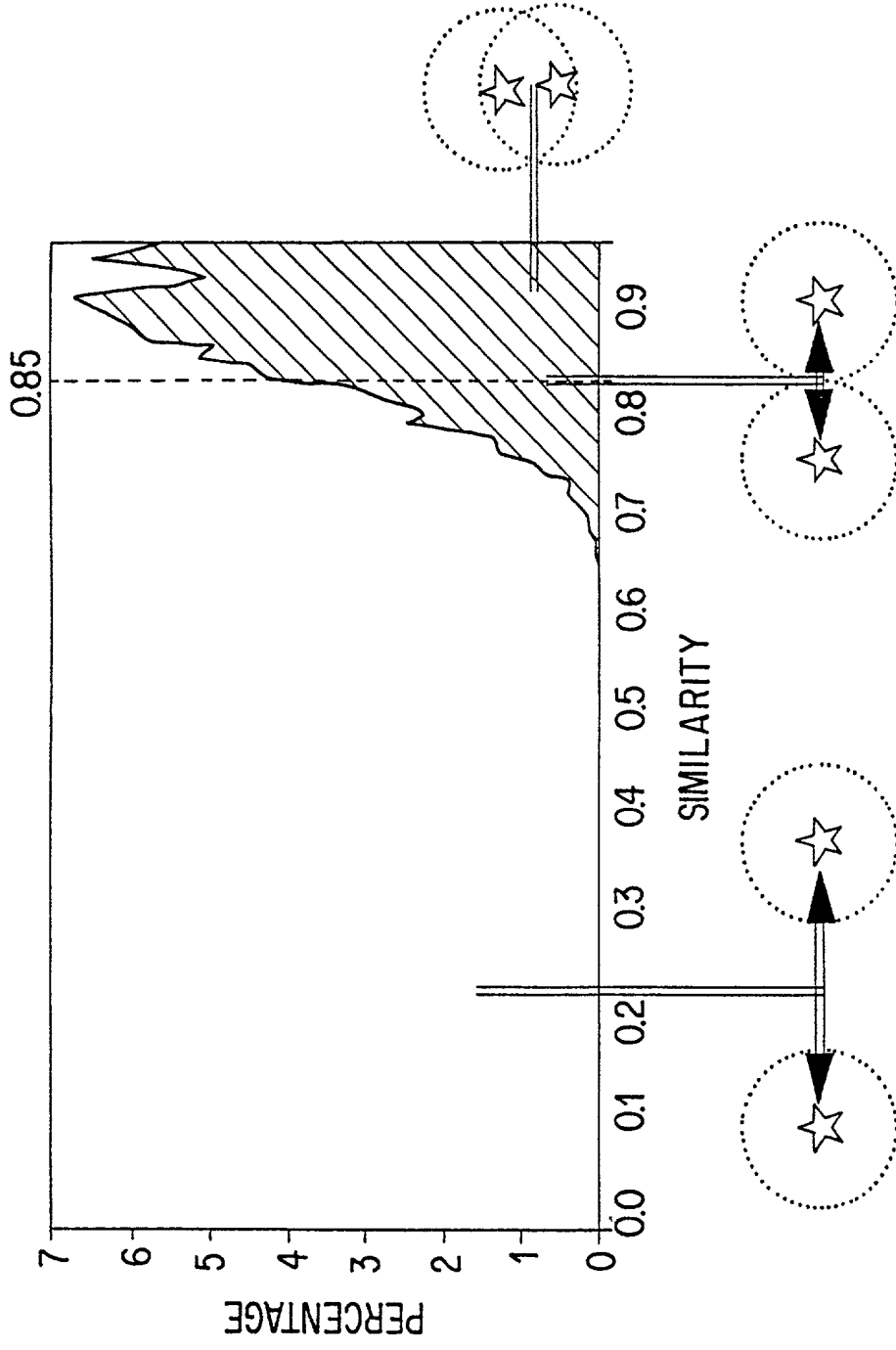


FIG. 13

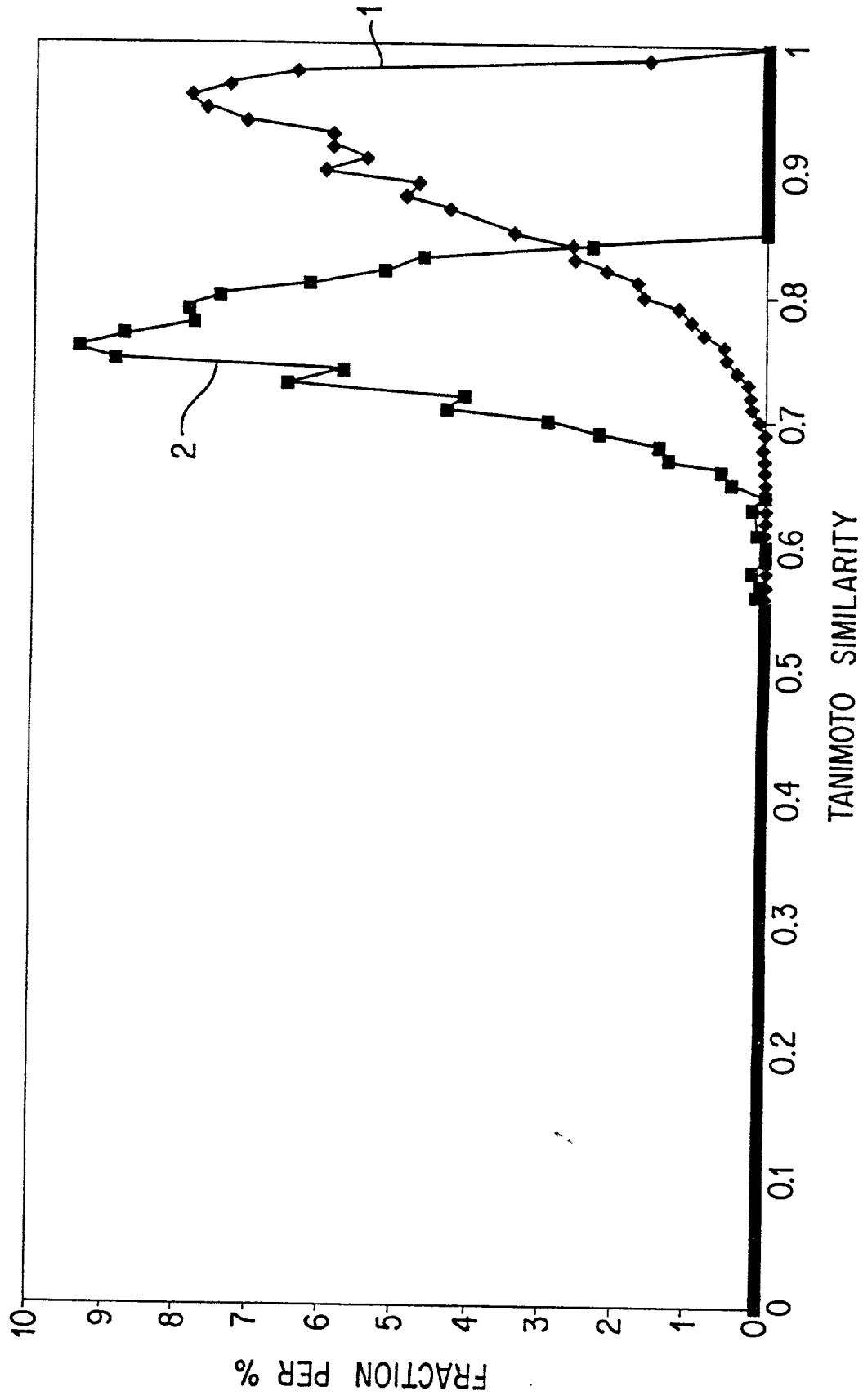


FIG.14

